

HEXANOIC ACID, 4-METHYLENE-, METHYL ESTER

Other names:	methyl 4-methylenehexanoate
Inchi:	InChI=1S/C8H14O2/c1-4-7(2)5-6-8(9)10-3/h2,4-6H2,1,3H3
InchiKey:	HREMKUVQMYGXPM-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=C(CC)CCC(=O)OC
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
af	0.4275		Cheméo Relay (1.0)
hf	-416.96	kJ/mol	Cheméo Relay (1.0)
hfus	16.67	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	427.74	K	Cheméo Relay (1.0)
tc	614.14	K	Cheméo Relay (1.0)
tf	196.29	K	Cheméo Relay (1.0)
vc	0.458	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.99	J/mol×K	455.29	Joback Method
cpg	274.81	J/mol×K	485.61	Joback Method
cpg	286.17	J/mol×K	515.92	Joback Method
cpg	297.08	J/mol×K	546.24	Joback Method
cpg	307.54	J/mol×K	576.55	Joback Method
cpg	317.57	J/mol×K	606.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73805488&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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